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Conformational analysis of 1,4-heterophosphinanes

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Abstract

Structure of 1,4-heterophosphinanes in solution was studied by the methods of dipole moments, Kerr effect, molecular mechanics, and density functional theory calculations. It was determined that chair conformation with an equatorial orientation of the exocyclic phenyl substituent is preferred for 1,4-heterophosphinanes independent of the second heteroatom in six-membered phosphorus heterocycle (oxygen, sulfur or silicon), and the coordination state of the phosphorus atom (σ3P or σ4P). Copyright © Taylor & Francis Group, LLC.

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Keywords

Conformational analysis, Dipole moments, Heterophosphinanes, Quantum chemical calculations